Pentanedioic acid, hexafluoro-
376-73-8 | DTXSID8059926

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.21 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.69e-01

Confidence level: 5.02e-01

Nearest Neighbors from the Training Set

Image not found
Acetic acid, trifluoro-
Measured: 8.77
Predicted: 4.36

Image not found
Fluoropanate-sodium
Measured: 1.31e-01
Predicted: 4.65e-01

Image not found
4-phosphonobutanoic Acid
Measured: 3.17
Predicted: 3.07

Image not found
3-Phosphonopropionic acid
Measured: 3.17
Predicted: 2.80

Image not found
Methyl phosphonic acid
Measured: 2.08e-01
Predicted: 3.13e-01